

```

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:CLASS 13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom

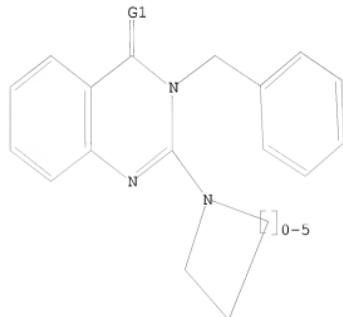
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L1 STRUCTURE UPLOADED

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L1 HAS NO ANSWERS
L1
      STR

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G1 O,S,N

Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SEARCH INITIATED 14:44:50 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 176 TO ITERATE

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100.0% PROCESSED 176 ITERATIONS
SEARCH TIME: 00.00.01
6 ANSWERS

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FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                      BATCH **COMPLETE**
PROJECTED ITERATIONS: 2725 TO 4315
PROJECTED ANSWERS: 6 TO 266

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L2 6 SEA SSS SAM L1

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=> s 11 sss full
FULL SEARCH INITIATED 14:44:57 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 3468 TO ITERATE

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100.0% PROCESSED 3468 ITERATIONS
SEARCH TIME: 00.00.01

127 ANSWERS

L3 127 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS
FULL ESTIMATED COST

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	185.88	186.10

FILE 'CAPLUS' ENTERED AT 14:45:02 ON 25 MAR 2009
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FILE COVERS 1907 - 25 Mar 2009 VOL 150 ISS 13
FILE LAST UPDATED: 24 Mar 2009 (20090324/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

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<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13
L4 4 L3
=> d ibib abs hitstr tot

LA ANSWER 1 OF 4 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 20081778800 CAPLUS

DOCUMENT NUMBER: 1491118693

TITLE: A potent, selective, bioavailable, and efficacious inhibitor of peptidyl peptidase IV. [Extraction to document cited in CAPLUS]

AUTHOR(S): Meng, Jun; Zhang, Shiyuan; Wallace, Michael B.; Stafford, Jeffrey A.; Kaldor, Stephen W.; Kasai, Daniel E.; Riviere, Marc; Shi, LibHong; Skene, Robert J.; Akaike, Toshiaki; Iwahashi, Keiji; Xu, Jungho; Wada, Toshiaki; Li, Dailey; Strickland, Michael

CORPORATE SOURCE: Takeda San Diego, Inc., San Diego, CA, 92121, USA

SOURCE: JOURNAL OF MEDICAL CHEMISTRY (2009), 51(14), 4257

CODE: JMMCA9 12891 001 2009 02 24 2009

PUBLISHER: AMERICAN CHEMICAL SOCIETY

DOCUMENT TYPE: Article

LANGUAGE: English

AB: On page 2287, Figure 1 is incorrect; the correct version of the figure is

IT 769157-45-3 94097-31-1 94097-31-1 94097-31-1

769157-45-3 94097-31-1 94097-31-1 94097-31-1

94097-93-1D 94098-01-0D 94098-01-0D 94098-01-0D

94098-01-0D 94098-01-0D 94098-01-0D 94098-01-0D

94098-07-4P

EL PAC (Pharmacological activity); FPK (Pharmacokinetics); SPM

18syn (preparation); TPS (Therapeutic use); MDC (Biological study); FREE

(Preparation); TPS (Biological study); FREE (Biological study)

769157-45-3 CAPLUS

CH Benzonitrile, 2-[(2R)-3-amino-1-piperidinyl]-7-fluoro-4-oxo-

2-[(2R)-3-amino-1-piperidinyl]-7-fluoro-4-oxo-3-(4-

-(4-quinazolinyl)methyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

NAME:

ON 1

CH 769157-44-4

CMF C21 H22 F NS O

Absolute stereochemistry.

LA ANSWER 1 OF 4 CAPLUS COPYRIGHT 2009 ACS on STN

(Continued)

14 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1491118693

TITLE: A potent, selective, bioavailable, and efficacious inhibitor of peptidyl peptidase IV. [Extraction to document cited in CAPLUS]

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94097-93-1D 94098-01-0D 94098-01-0D 94098-01-0D

94098-01-0D 94098-01-0D 94098-01-0D 94098-01-0D

94098-07-4P

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-(4-quinazolinyl)methyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

NAME:

ON 1

CH 769157-44-4

CMF C21 H22 F NS O

Absolute stereochemistry.

LA ANSWER 1 OF 4 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)

CH Benzonitrile, 2-[(2R)-3-amino-1-piperidinyl]-7-fluoro-4-oxo-

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-(4-quinazolinyl)methyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

NAME:

ON 1

CH 769157-44-4

CMF C21 H22 F NS O

Absolute stereochemistry.

LA ANSWER 1 OF 4 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)

CH Benzonitrile, 2-[(2R)-3-amino-1-piperidinyl]-7-fluoro-4-oxo-

2-[(2R)-3-amino-1-piperidinyl]-7-fluoro-4-oxo-3-(4-

-(4-quinazolinyl)methyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

NAME:

ON 1

CH 769157-44-4

CMF C21 H22 F NS O

Absolute stereochemistry.

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94098-01-0D 94098-01-0D 94098-01-0D 94098-01-0D

94098-07-4P

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Absolute stereochemistry.

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NAME:

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Absolute stereochemistry.

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EL PAC (Pharmacological activity); FPK (Pharmacokinetics); SPM

18syn (preparation); TPS (Therapeutic use); MDC (Biological study); FREE

(Preparation); TPS (Biological study); FREE (Biological study)

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Absolute stereochemistry.

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EL PAC (Pharmacological activity); FPK (Pharmacokinetics); SPM

18syn (preparation); TPS (Therapeutic use); MDC (Biological study); FREE

(Preparation); TPS (Biological study); FREE (Biological study)

NAME:

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CH 769157-44-4

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Absolute stereochemistry.

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94098-07-4P

EL PAC (Pharmacological activity); FPK (Pharmacokinetics); SPM

18syn (preparation); TPS (Therapeutic use); MDC (Biological study); FREE

(Preparation); TPS (Biological study); FREE (Biological study)

NAME:

ON 1

CH 769157-44-4

CMF C21 H22 F NS O

Absolute stereochemistry.

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94098-01-0D 94098-01-0D 94098-01-0D 94098-01-0D

94098-07-4P

EL PAC (Pharmacological activity); FPK (Pharmac

14 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)

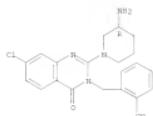
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 CHN 76-05-1
 CNF C2 H F3 O2



225 942907-97-1 CAPLUS
 Benzotriazole, 2-[(2-[(2S)-3-amino-1-piperidinyl]-8-chloro-4-oxo-3(4H)-quinoxolinyl)methyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

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 CHN 942907-96-9
 CNF C11 H29 Cl1 N3 O

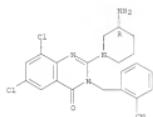
Absolute stereochemistry.



CH 2
 CHN 76-05-1
 CNF C2 H F3 O2



14 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)



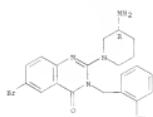
CH 2
 CHN 76-05-1
 CNF C2 H F3 O2



225 942908-01-0 CAPLUS
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CH 1
 CHN 769157-89-7
 CNF C11 H29 Br1 N3 O

Absolute stereochemistry.



CH 2

Habte

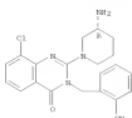
03/25/2009

14 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)

225 942907-98-2 CAPLUS
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CH 1
 CHN 942907-98-2
 CNF C11 H29 Cl1 N3 O

Absolute stereochemistry.



CH 2
 CHN 76-05-1
 CNF C2 H F3 O2



225 942908-00-9 CAPLUS
 Benzotriazole, 2-[(2-[(2S)-3-amino-1-piperidinyl]-6,8-dichloro-4-oxo-3(4H)-quinoxolinyl)methyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

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Absolute stereochemistry.



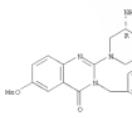
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 CHN 76-05-1
 CNF C2 H F3 O2



225 942908-02-0 CAPLUS
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 CNF C12 H23 N3 O2

Absolute stereochemistry.

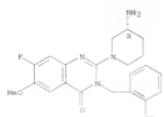


CH 2
 CHN 76-05-1
 CNF C2 H F3 O2



225 942908-03-2 CAPLUS
 Benzotriazole, 2-[(2-[(2S)-3-amino-1-piperidinyl]-6,7-dimethoxy-4-oxo-3(4H)-quinoxolinyl)methyl]- (CA INDEX NAME)

Absolute stereochemistry.



OH 2

CN 74-05-1
CMF C2 H F3 O2

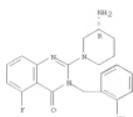
30 749157-79-3 CAPLOS

32 Benzonitrile, 2-[(2-[(3R)-3-amino-1-piperidinyl]-5-fluoro-4-oxo-3-(4R)-quinalidinyl)methyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CN 1

CN 769157-79-2
CMF C21 H20 F NS O

Absolute stereochemistry.



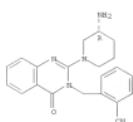
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CMF C2 H F3 O2

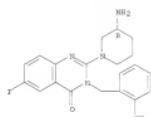
30 940907-93-7 CAPLOS

32 Benzonitrile, 2-[(2-[(3R)-3-amino-1-piperidinyl]-4-oxo-3-(4R)-quinalidinyl)methyl]- (CA INDEX NAME)

Absolute stereochemistry.

30 940907-94-8 CMF 08
32 Benzonitrile, 2-[(2-[(3R)-3-amino-1-piperidinyl]-4-oxo-3-(4R)-quinalidinyl)methyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)CN 1
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Absolute stereochemistry.



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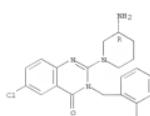
30 940907-95-9 CAPLOS

32 Benzonitrile, 2-[(2-[(3R)-3-amino-1-piperidinyl]-6-chloro-4-oxo-3-(4R)-quinalidinyl)methyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

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CN 769157-63-3
CMF C21 H20 Cl NS O

Absolute stereochemistry.



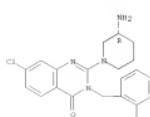
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CN 74-05-1
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32 Benzonitrile, 2-[(2-[(3R)-3-amino-1-piperidinyl]-7-chloro-4-oxo-3-(4R)-quinalidinyl)methyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

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Absolute stereochemistry.



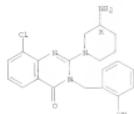
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14 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)
 CHN 76-05-1
 CMF C2 H F3 O2



382 940907-99-3 CAPLUS
 Benzonitrile, 2-[2-[(3R)-3-amino-1-piperidinyl]-8-chloro-4-oxo-3(4H)-
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Absolute stereochemistry.

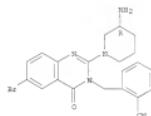


CN 2
 CHN 76-05-1
 CMF C2 H F3 O2



382 940908-00-9 CAPLUS
 Benzonitrile, 2-[2-[(3R)-3-amino-1-piperidinyl]-4,8-dichloro-4-oxo-3(4H)-

14 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)



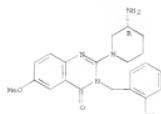
CN 2
 CHN 76-05-1
 CMF C2 H F3 O2



382 940908-01-1 CAPLUS
 Benzonitrile, 2-[2-[(3R)-3-amino-1-piperidinyl]-8-methoxy-4-oxo-3(4H)-
 quinazolinyl]methyl-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CN 1
 CHN 769157-93-3
 CMF C21 H21 N5 O2

Absolute stereochemistry.



CN 2

Habte

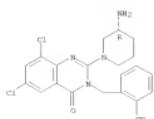
03/25/2009

14 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)
 quinazolinyl)methyl-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CN 1

CHN 769157-92-8
 CMF C21 H19 C12 N5 O

Absolute stereochemistry.



CN 2

CHN 76-05-1
 CMF C2 H F3 O2



382 940908-01-0 CAPLUS
 Benzonitrile, 2-[2-[(3R)-3-amino-1-piperidinyl]-8-bromo-4-oxo-3(4H)-
 quinazolinyl]methyl-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CN 1

CHN 769157-99-3
 CMF C21 H20 N5 O

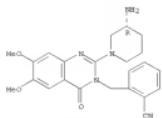
Absolute stereochemistry.

14 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)
 CHN 76-05-1
 CMF C2 H F3 O2



382 940908-01-2 CAPLUS
 Benzonitrile, 2-[2-[(3R)-3-amino-1-piperidinyl]-6,7-dimethoxy-4-oxo-3(4H)-
 quinazolinyl]methyl- (CA INDEX NAME)

Absolute stereochemistry.



382 940908-04-4 CAPLUS
 Benzonitrile, 2-[2-[(3R)-3-amino-1-piperidinyl]-8-methoxy-4-oxo-3(4H)-
 quinazolinyl]methyl-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CN 1

CHN 940908-04-3
 CMF C21 H23 N5 O2

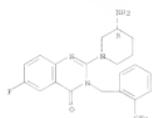
Absolute stereochemistry.

14 ANSWER 3 OF 4 CAPLOS COPYRIGHT 2009 ACS on STN (Continued)
 CH3 76-05-1
 CHF2 C2 H F3 O2



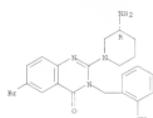
320 769157-81-5 CAPLOS
 CH3 4178-(Quinazolin-2-yl)-2-[(3R)-3-amino-1-piperidinyl]-4-fluoro-3-[(2-
 (trifluoromethyl)phenyl)methyl]- (CA INDEX NAME)

Absolute stereochemistry.

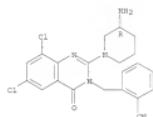


320 769157-89-3 CAPLOS
 CH3 Benzonicitrile, 2-[(2-[(3R)-3-amino-1-piperidinyl]-6-bromo-4-oxo-3-(4R)-
 quinazolinyl)methyl]- (CA INDEX NAME)

Absolute stereochemistry.

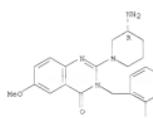


14 ANSWER 3 OF 4 CAPLOS COPYRIGHT 2009 ACS on STN (Continued)



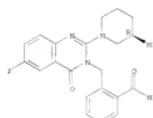
320 769157-93-9 CAPLOS
 CH3 Benzonicitrile, 2-[(2-[(3R)-3-amino-1-piperidinyl]-6-methoxy-4-oxo-3-(4R)-
 quinazolinyl)methyl]- (CA INDEX NAME)

Absolute stereochemistry.



320 769157-94-0 CAPLOS
 CH3 Benzonic acid, 2-[(2-[(3R)-3-amino-1-piperidinyl]-6-fluoro-4-oxo-3-(4R)-
 quinazolinyl)methyl]- (CA INDEX NAME)

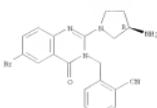
Absolute stereochemistry.



14 ANSWER 3 OF 4 CAPLOS COPYRIGHT 2009 ACS on STN (Continued)
 CH3 769157-93-7 CAPLOS

CH3 Benzonic acid, 2-[(2-[(3R)-3-amino-1-piperidinyl]-4-bromo-4-oxo-3-(4R)-
 quinazolinyl)methyl]- (CA INDEX NAME)
 CH3 1
 CH3 769157-99-6
 CHF2 C2 H3 N5 O

Absolute stereochemistry.



CH3 2

CH3 76-05-1
 CHF2 C2 H F3 O2

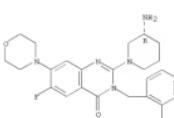


320 769157-92-8 CAPLOS
 CH3 Benzonic acid, 2-[(2-[(3R)-3-amino-1-piperidinyl]-6,8-dichloro-4-oxo-3-(4R)-
 quinazolinyl)methyl]- (CA INDEX NAME)

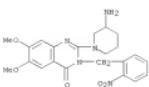
Absolute stereochemistry.

14 ANSWER 3 OF 4 CAPLOS COPYRIGHT 2009 ACS on STN (Continued)
 CH3 769157-95-1 CAPLOS
 CH3 Benzonic acid, 2-[(2-[(3R)-3-amino-1-piperidinyl]-6-fluoro-7-(4-
 morpholinyl)-4-oxo-3-(4R)-quinazolinyl)methyl]- (CA INDEX NAME)

Absolute stereochemistry.



320 769158-01-2 CAPLOS
 CH3 4-(2H)-Quinazolinede, 2-[(3R)-3-amino-1-piperidinyl]-6,7-dimethoxy-3-[(2-
 nitrophenyl)methyl]- (CA INDEX NAME)



320 769158-02-3 CAPLOS
 CH3 Benzonic acid,
 2-[(2-[(3R)-3-amino-1-piperidinyl]-6,7-dimethoxy-4-oxo-3-(4R)-
 quinazolinyl)methyl]-, ethyl ester (CA INDEX Name)

Absolute stereochemistry.

